

12/10/03

09/995,609

=> s l1 full

FULL SEARCH INITIATED 11:29:34 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1843 TO ITERATE

100.0% PROCESSED 1843 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

L5 1 SEA SSS FUL L1

=> s l2 full

FULL SEARCH INITIATED 11:29:38 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1843 TO ITERATE

100.0% PROCESSED 1843 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

L6 1 SEA SSS FUL L2

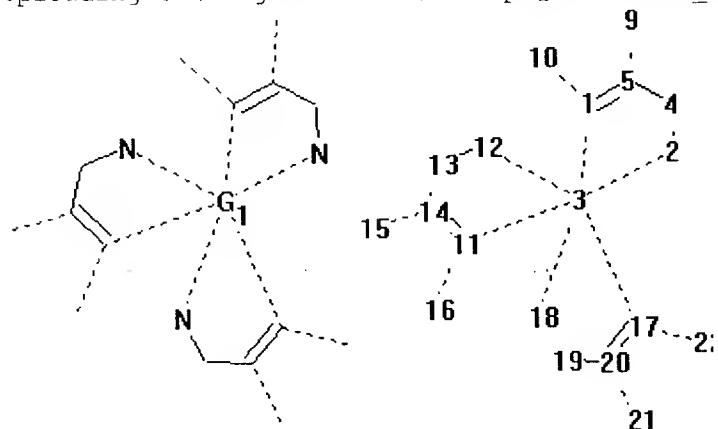
L11 0 S L6 NOT L5

Search
HISTORIES

12/10/03

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Uploading C:\Program Files\Stnexp\Queries\09_995609 n_3 chain only.str



chain nodes :

9 10 15 16 21 22

ring nodes :

1 2 3 4 5 11 12 13 14 17 18 19 20

chain bonds :

1-10 5-9 11-16 14-15 17-22 20-21

ring bonds :

1-3 1-5 2-4 2-3 3-12 3-11 3-18 3-17 4-5 11-14 12-13 13-14 17-20
18-19
19-20

exact/norm bonds :

1-3 1-5 1-10 2-4 2-3 3-12 3-11 3-18 3-17 4-5 5-9 11-14 11-16 12-13
13-14 14-15 17-20 17-22 18-19 19-20 20-21

G1:Ir,Rh

Connectivity :

2:3 M minimum R ring 12:3 M minimum R ring 18:3 M minimum R ring

Match level :

1:Atom 2:CLASS 3:Atom 4:Atom 5:Atom 9:CLASS 10:CLASS 11:Atom 12:CLASS
13:Atom
14:Atom 15:CLASS 16:CLASS 17:Atom 18:CLASS 19:Atom 20:Atom 21:CLASS
22:CLASS

L1 STRUCTURE UPLOADED

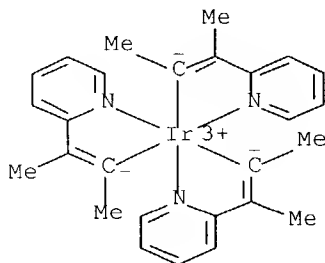
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L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 594819-53-1 REGISTRY
 ED Entered STN: 29 Sep 2003
 CN Iridium, tris[1-methyl-2-(2-pyridinyl-κN)-1-propenyl-κC]-
 (9CI) (CA INDEX NAME)
 MF C27 H30 Ir N3
 CI CCS
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3IrN-C3IrN-	IrNC3-IrNC3-	5-5-5-6-6-6	C21IrN3	9762.174.1	1
C3IrN-C5N-	IrNC3-NC5-				
C5N-C5N	NC5-NC5				



1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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L1 FILE 'REGISTRY' ENTERED AT 13:53:42 ON 10 DEC 2003
SCREEN 2049 AND 1838

FILE 'STNGUIDE' ENTERED AT 13:54:38 ON 10 DEC 2003

L2 FILE 'REGISTRY' ENTERED AT 13:54:50 ON 10 DEC 2003
L3 SCREEN 2049 AND 1838
L4 QUE SCREEN
L5 STRUCTURE UPLOADED
L6 1 S L2 AND L4
L7 18 S L2 AND L4 FULL
L8 320037 S (PT OR IR OR RH OR PD)/ELS
0 S L6 AND L7

FILE 'STNGUIDE' ENTERED AT 13:59:26 ON 10 DEC 2003

L9 FILE 'REGISTRY' ENTERED AT 14:05:01 ON 10 DEC 2003
L10 STRUCTURE UPLOADED
L11 0 S L9
42 S L9 FULL

FILE 'STNGUIDE' ENTERED AT 14:06:26 ON 10 DEC 2003

L12 FILE 'REGISTRY' ENTERED AT 14:18:07 ON 10 DEC 2003
10 S L11 AND (C57 H69 CL3 IR N3 OR C36 H56 N2 O2 PT OR C33 H42 IR

L13 FILE 'HCAPLUS, GMELIN, MARPAT' ENTERED AT 14:19:01 ON 10 DEC 2003
L14 8 S L11
8 S L11

L15 FILE 'REGISTRY' ENTERED AT 14:23:43 ON 10 DEC 2003
SEL L12 1- RN : 10 TERMS

L16 FILE 'HCAPLUS, GMELIN, MARPAT' ENTERED AT 14:24:04 ON 10 DEC 2003
2 S L15

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FILE 'HCAPLUS' ENTERED AT 13:23:34 ON 10 DEC 2003

L1 7 S E4-E6
 E THOMPSON M/IN
L2 1 S E4
 E THOMPSON MARK/IN
 E THOMPSON M/IN
L3 4 S E3
 E THOMPSON MARK/IN
L4 60 S E3,E6
L5 65 S L2-L4
L6 5 S L1 AND L5
L7 SEL L6 1- RN IC : 188 TERMS
L8 578535 S L7
L9 5 S L8 AND L6

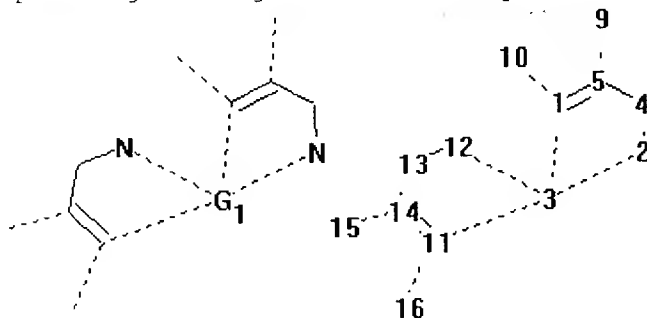
*The vinyl pyridine ligand
was not indexed for Thompson*

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FILE 'REGISTRY' ENTERED AT 14:45:05 ON 10 DEC 2003

 \Rightarrow

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chain nodes :

9 10 15 16

ring nodes :

1 2 3 4 5 11 12 13 14

chain bonds :

1-10 5-9 11-16 14-15

ring bonds :

1-3 1-5 2-4 2-3 3-12 3-11 4-5 11-14 12-13 13-14

exact/norm bonds :

1-3 1-5 1-10 2-4 2-3 3-12 3-11 4-5 5-9 11-14 11-16 12-13 13-14
14-15

$$\text{G1: Pd, Pt}$$

Connectivity :

2:3 M minimum R ring 12:3 M minimum R ring

Match level :

```
1:Atom 2:CLASS 3:Atom 4:Atom 5:Atom 9:CLASS 10:CLASS 11:Atom 12:CLASS
```

13:Atom

```
14:Atom  15:CLASS  16:CLASS
```

L17 STRUCTURE UPLOADED

L18 0 SEA SSS SAM L17

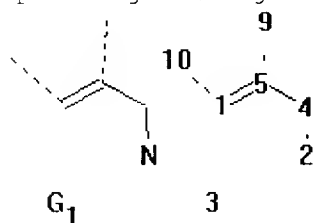
L19 0 SEA SSS FUL L17

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```

L1          320037 S (PT OR PD OR IR OR RH)/ELS
L2          361912 S (PYRIDIN? OR QUINOL? OR PYAZO? OR BENZOTHTIAZO? OR
BENZOXAZO?
L3          3786 S L1(P)L2
L4          154792 S N/ELS(P)L1
L5          SCREEN 2049
L6          3501 S L3 AND L4
L7          2605 S NC=1 AND L6
L8          1386 S C3IRN/EAS
L9          50 S L7 AND L8
L10         0 S IRNC3/EAS
L11         1365 S IRNC3/ESS
L12         47 S L11 AND L9
L13         3956879 S 3/CNRS
L14         2 S L12 AND L13
L15         1743838 S 4/CNRS
L16         0 S (PT OR PD)/ELS AND L2 AND L8 AND NC=1 AND L11 AND L15
L17         0 S (PT OR PD)/ELS AND (C3NPD OR C3NPD)/EAS AND NC=1 AND (PTNC3
O
L18         613 S (PT OR PD)/ELS AND (C3NPD OR C3NPD)/EAS AND NC=1 AND 4/CNRS
Uploading C:\Program Files\Stnexp\Queries\09 995609 n 2 chain not bonded.str

```



```
chain nodes :
1 3 5 9 10
ring nodes :
2 4
chain bonds :
1-10 1-5 4-5 5-9
ring bonds :
2-4
exact/norm bonds :
1-10 2-4 5-9
exact bonds :
1-5 4-5
```

G1: Pd, Pt

```
Connectivity :
2:1 E exact R ring
Match level :
1:Atom 2:CLASS 3:Atom 4:Atom 5:Atom 9:CLASS 10:CLASS
```

```

L20      STRUCTURE  UPLOADED
L21              0 SEA SSS SAM L20
L22              0 SEA SSS FUL L20

```

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(FILE 'REGISTRY' ENTERED AT 14:45:05 ON 10 DEC 2003)

L1 213739 S (PT OR PD)/ELS
L2 QUE N/ELS AND L1
L3 0 CHELATE? AND L2
L4 0 COORDINAT? AND L2
L5 44036 COMPLEX AND L2
L6 2844616 PYRIDIN? OR QUINOLIN? OR IMIDAZO? OR PYAZOL? OR BENZOTHIAZOL?
OR BENZOXAZOL? OR BENZIMIDAZOL?
L7 8657 L5 AND L6
L8 0 L1(P)N/ELS(P)COMPLEX(P)L6
L9 1869 VINYL PYRIDIN?
L10 4 L9 AND L7

FILE 'MARPAT, HCAPLUS, GMELIN' ENTERED AT 15:07:13 ON 10 DEC 2003

L11 8 S L10

FILE 'MARPAT, HCAPLUS, GMELIN' ENTERED AT 15:30:35 ON 10 DEC 2003

L12 441228 S PYRIDIN? OR QUINOLIN? OR IMIDAZO? OR PYAZOL? OR BENZOTHIAZOL?
L13 1675179 S CHELAT? OR COORDINAT? OR COMPLEX?
L14 43674 S L12 (10A)L13
L15 1051924 S PT OR RH OR IR OR PD OR PALLADIUM OR RHENIUM OR IRIIDIUM OR PL
L16 4302 S L14(10A)L15
L17 622282 S VINYL? OR ETHEN? OR ALLYL?
L18 127 S L16(10A)L17
L19 49 S VINYL?(10A)L16
L20 33 S PYRAZOL?(10A)L13(10A)L15(10A)L17
L21 32 S L20 NOT L19
L22 SEL L21 12 RN : 18 TERMS
L23 5651 S L22
L24 3 S L21 AND L2

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FYI

L10 ANSWER 1 OF 4: REGISTRY COPYRIGHT 2003 ACS on STN

RN 116745-83-6 REGISTRY

CN Palladium, dichlorobis(2-ethenylpyridine)-, (SP-4-1)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

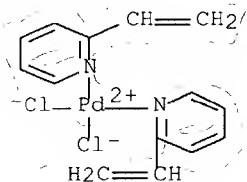
CN Pyridine, 2-ethenyl-, palladium complex

OTHER NAMES:

CN trans-Dichlorobis(2-vinylpyridine)palladium

MF C14 H14 Cl2 N2 Pd

LC STN Files: CA, CAPLUS, CASREACT



2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)